**Power-to-Syngas Processes by Reactor-Separator Superstructure Optimization**

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**Highlights**

* Power-to-Syngas process superstructure for different syngas compositions introduced.
* Optimal energy pathways to syngas from renewables identified via LP.

**1. Introduction**

The transition from fossil (coal, oil, gas) to renewable feedstock and energy carriers (solar, wind, water, biomass) has become a matter of uttermost importance in the chemical industries. Moreover, the current large CO2 emissions represent both a threat for the climate and an opportunity for an alternative carbon source. Schack et al. [1] showed how the shift towards sustainable production scenarios could be accomplished by identifying well-suited target products. In this regard, syngas is an ideal candidate: as reported by Wenzel et al. [2], it bridges the inputs from renewables and state-of-the-art downstream processes to fuels and chemicals by adjustment of the H2/CO ratio. Reactor-separator processes are the tool allowing for such bridging. Different process alternatives available in this context suggest the deployment of a superstructural representation wherein different technologies can be embedded. Categories of available separation methods to purify and adjust the syngas to the requirements of the desired downstream processes include membrane separation, pressure swing adsorption, scrubbing and cryogenic operations.

**2. Methods**

In our superstructure approach, different types of catalytic conversion steps and separation methods are combined. The superstructure is the basis for the formulation of a Linear Program (LP) used for process optimization. The complexity of the system is reduced by assuming Gibbs reactors and sharp-split separation tasks. As shown in Figure 1, the feedstocks considered are water and biomass. The most promising reactor technologies considered are reverse water gas shift (RWGS) and steam reforming of methane (SR).



Figure 1 Schematic representation of a syngas plant. Biomass and water are converted into the reactants required for the generation of the final product.

The first objective to be minimized is the total energy requirement. Furthermore, pseudo prices are applied to the variables in the objective function to allow for the differentiation between day and night plant operations, therefore accounting for the intermittency of the renewable power sources. The solutions depend on the hydrogen to carbon monoxide ratio which the syngas must fulfil to meet the product specification.

**3. Results and discussion**

Preliminary results indicate that, for RWGS, the optimal syngas production route consists of water removal followed by a sequence of pressure swing adsorption steps for the adjustment of the hydrogen to carbon monoxide ratio. This approach is extended to scenarios where SR is included in the same optimization problem. Water electrolysis proves to be a bottleneck for the syngas production, possibly mitigated by the synergy between SR, yielding a high H2/CO ratio, and RWGS.

**4. Conclusions**

The derivation of the method presented in this work is motivated by the need for an effective screening tool to identify the most energy efficient process within a large number of alternatives. The energy efficiency is of foremost importance in the context of Power-to-Chemical conversion systems, where the energy and raw chemicals are to be supplied from renewable sources. Nevertheless, this approach does not contrast with economic based optimizations but it offers a complementary standpoint.

**References**

1. D. Schack, L. Rihko-Struckmann, K. Sundmacher, Ind. Eng. Chem. Res. 57 (2018) 9889–9902.
2. M. Wenzel, L. Rihko-Struckmann, K. Sundmacher, AIChE Journal, 63 (2017) 15-22.